Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for:

The effects of different heterocycles and solvents on the ESIPT mechanisms for three novel photoactive mono-formylated benzoxazole derivatives

Jiaojiao Hao, Yang Yang*[a]

State Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

E-mail: light_yang@dicp.ac.cn

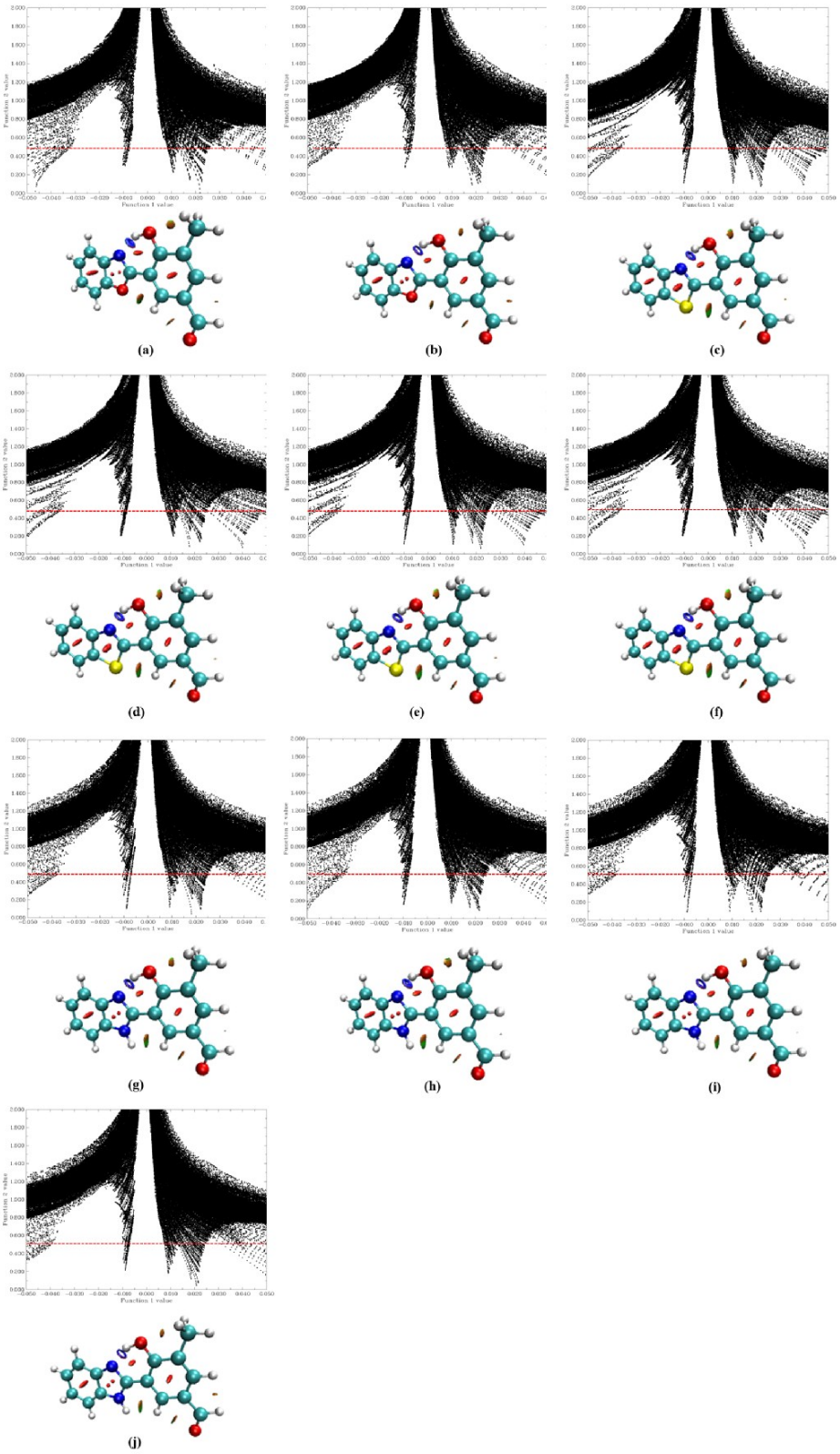

Figure S1. The RDG isosurfaces for compound **A-C** in the S_0 and S_1 states on polar 1,4-dioxane or nonpolar dichloromethane solvents. Here, in dichloromethane on S_0 state for **A** (a), **B** (e) and **C** (i); in 1,4-dioxane on S_0 state for **B** (c) and **C** (g); in dichloromethane on S_1 state for **A** (b), **B** (f) and **C** (j); in 1,4-dioxane on S_1 state for **B** (d) and **C** (h).

Table S1. Cartesian coordinates of structures **A-C** in S_0 and S_1 states in polar 1,4-dioxane solvent.

1. A (S_0)				
Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-4.93742	0.983929	-0.000139
6	0	-5.048802	-0.414455	-0.000226
6	0	-3.927624	-1.23662	-0.00022
6	0	-2.68338	-0.612209	-0.000122
6	0	-2.599072	0.781664	-0.000038
6	0	-3.696879	1.618627	-0.000043
7	0	-1.387077	-1.119743	-0.00009
6	0	-0.605575	-0.076339	0.000018
8	0	-1.264446	1.120337	0.000039
6	0	0.84187	-0.09282	0.000065
6	0	1.516555	-1.343713	0.000077
6	0	2.924404	-1.395207	0.000077
6	0	3.619932	-0.198807	0.000069
6	0	2.970736	1.045801	0.000071
6	0	1.58118	1.088293	0.00007
8	0	0.857066	-2.509697	0.000139
6	0	3.617269	-2.729183	0.000092
6	0	3.766426	2.281428	0.000069
8	0	3.313766	3.409145	0.000042
1	0	-5.83684	1.586084	-0.000149
1	0	-6.034409	-0.862124	-0.0003
1	0	-4.012729	-2.315074	-0.000287
1	0	-3.599362	2.695497	0.000022
1	0	4.704936	-0.22309	0.000071
1	0	1.078819	2.046304	0.000058
1	0	-0.119049	-2.33348	0.000229
1	0	3.338374	-3.318654	-0.876294
1	0	4.699378	-2.601046	0.000215
1	0	3.33818	-3.318736	0.876358
1	0	4.863445	2.121898	0.00004

2. A (S_1)				
Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-4.936465	0.985617	-0.000153
6	0	-5.049462	-0.412351	-0.000252
6	0	-3.928856	-1.235794	-0.000245
6	0	-2.683275	-0.613833	-0.000133
6	0	-2.597252	0.780063	-0.000036
6	0	-3.694332	1.617987	-0.000042
7	0	-1.388851	-1.124105	-0.000096

6	0	-0.603361	-0.082729	0.000032
8	0	-1.262911	1.116712	0.000051
6	0	0.844043	-0.097032	0.000083
6	0	1.51146	-1.344566	0.000089
6	0	2.929879	-1.39006	0.000064
6	0	3.632031	-0.211935	0.000053
6	0	2.988256	1.06603	0.000071
6	0	1.57111	1.094392	0.000087
8	0	0.85857	-2.522931	0.000178
6	0	3.619156	-2.727055	0.000074
6	0	3.753517	2.233041	0.000062
8	0	3.303588	3.454557	0.000053
1	0	-5.834949	1.589249	-0.000164
1	0	-6.035575	-0.859075	-0.000337
1	0	-4.015461	-2.314184	-0.000323
1	0	-3.595612	2.694834	0.000032
1	0	4.715595	-0.248394	0.00004
1	0	1.044333	2.037245	0.000082
1	0	-0.115637	-2.351006	0.000305
1	0	3.337313	-3.315169	-0.876213
1	0	4.701899	-2.603001	0.000072
1	0	3.337315	-3.315158	0.876369
1	0	4.85007	2.196035	0.000039

3. B (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-5.165346	-0.491697	-0.000162
6	0	-4.970058	0.896263	-0.000172
6	0	-3.69459	1.436396	-0.000139
6	0	-2.597723	0.570013	-0.000097
6	0	-2.805786	-0.823653	-0.000087
6	0	-4.087126	-1.366389	-0.00012
7	0	-1.270287	0.951618	-0.00006
6	0	-0.451664	-0.063032	-0.000022
16	0	-1.255621	-1.651927	-0.000033
6	0	0.998321	0.084246	0.000027
6	0	1.574543	1.387272	0.000061
6	0	2.974617	1.556172	0.000118
6	0	3.770538	0.425409	0.000134
6	0	3.225906	-0.868117	0.000096
6	0	1.844826	-1.02281	0.000043
8	0	0.82545	2.495325	0.000042
6	0	3.550198	2.944921	0.000156
6	0	4.116135	-2.036299	0.000114
8	0	3.752752	-3.196437	0.000091

1	0	-6.171864	-0.890295	-0.000188
1	0	-5.829461	1.554542	-0.000205
1	0	-3.533857	2.506636	-0.000146
1	0	-4.242209	-2.437243	-0.000113
1	0	4.849661	0.540961	0.000176
1	0	1.441979	-2.028423	0.000014
1	0	-0.133835	2.225378	-0.000004
1	0	4.639334	2.909801	0.000221
1	0	3.221278	3.508315	0.876322
1	0	3.221385	3.508318	-0.87605
1	0	5.197166	-1.791771	0.000163

4. B (S_1)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-5.161486	-0.523204	-0.000168
6	0	-4.993277	0.868401	-0.000192
6	0	-3.734626	1.423358	-0.000156
6	0	-2.623163	0.57103	-0.000094
6	0	-2.794144	-0.813431	-0.000072
6	0	-4.073778	-1.368887	-0.00011
7	0	-1.256465	0.994414	-0.000041
6	0	-0.466069	-0.045769	0.000032
16	0	-1.247234	-1.617998	-0.000019
6	0	1.016692	0.110197	0.000069
6	0	1.580673	1.394224	0.000087
6	0	2.990709	1.534119	0.000096
6	0	3.782572	0.4144	0.000095
6	0	3.233364	-0.886223	0.000085
6	0	1.854299	-1.012624	0.000074
8	0	0.84176	2.55594	0.000111
6	0	3.585738	2.937858	0.000116
6	0	4.127702	-2.049832	0.000111
8	0	3.667151	-3.274806	-0.000007
1	0	-6.162021	-0.937285	-0.0002
1	0	-5.865904	1.50877	-0.000238
1	0	-3.592668	2.49671	-0.000171
1	0	-4.211126	-2.442896	-0.000098
1	0	4.859492	0.524894	0.000103
1	0	1.409349	-1.998419	0.00006
1	0	-0.107025	2.255696	0.000143
1	0	4.670119	2.893859	0.000087
1	0	3.261341	3.492984	0.877242
1	0	3.261295	3.493028	-0.876965
1	0	5.205623	-1.931052	-0.000038

5. C (S_0)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	5.059615	-0.491672	-0.002375
6	0	5.025032	0.913496	0.002795
6	0	3.824357	1.611011	0.005359
6	0	2.659028	0.851266	0.002618
6	0	2.678797	-0.559211	-0.002558
6	0	3.894783	-1.244197	-0.00512
7	0	1.318741	1.1924	0.003621
6	0	0.591931	0.02942	-0.000597
7	0	1.380307	-1.033299	-0.004332
6	0	-0.86271	-0.048601	-0.000889
6	0	-1.48774	-1.32792	0.00043
6	0	-2.893641	-1.440876	0.001903
6	0	-3.645548	-0.27958	0.001302
6	0	-3.050529	0.990847	-0.000781
6	0	-1.662675	1.089944	-0.001983
8	0	-0.779388	-2.461471	0.000356
6	0	-3.523942	-2.80549	0.003749
6	0	-3.889595	2.194016	-0.001765
8	0	-3.476687	3.338727	-0.003564
1	0	6.018622	-0.994143	-0.004305
1	0	5.956628	1.465073	0.004772
1	0	3.801323	2.69317	0.00923
1	0	3.918697	-2.32619	-0.009157
1	0	0.946333	2.127728	0.00945
1	0	-4.728403	-0.352565	0.002269
1	0	-1.230129	2.082691	-0.004314
1	0	0.195071	-2.228195	-0.001844
1	0	-4.610902	-2.727568	0.005089
1	0	-3.218609	-3.382292	-0.872266
1	0	-3.216354	-3.380962	0.879845
1	0	-4.980005	1.996771	-0.000653

6. C (S_1)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	5.048109	-0.477371	0.000032
6	0	4.992242	0.942787	0.000468
6	0	3.786748	1.632023	0.000553
6	0	2.631254	0.862555	0.000194
6	0	2.666179	-0.57994	-0.000237
6	0	3.908338	-1.24889	-0.000327
7	0	1.304152	1.182704	0.0001
6	0	0.572505	0.001436	-0.000226

7	0	1.412546	-1.070037	-0.000539
6	0	-0.83215	-0.066733	-0.000383
6	0	-1.47113	-1.343808	-0.00014
6	0	-2.890807	-1.445927	0.000275
6	0	-3.621132	-0.275856	0.000375
6	0	-3.033458	1.015689	0.000003
6	0	-1.640943	1.123471	-0.000466
8	0	-0.783324	-2.487989	-0.000222
6	0	-3.53605	-2.802658	0.000577
6	0	-3.889031	2.195074	-0.000002
8	0	-3.455786	3.359915	-0.000265
1	0	6.018807	-0.955829	-0.000034
1	0	5.919679	1.500309	0.000722
1	0	3.7537	2.712971	0.000872
1	0	3.946465	-2.329513	-0.000668
1	0	0.912202	2.110833	0.000814
1	0	-4.705026	-0.339338	0.000701
1	0	-1.203922	2.111045	-0.001221
1	0	0.192011	-2.282399	-0.000685
1	0	-4.621761	-2.707941	0.00073
1	0	-3.242552	-3.386197	-0.876008
1	0	-3.242291	-3.385928	0.877257
1	0	-4.975371	1.996798	0.000313

Table S2. Cartesian coordinates of structures **A-C** in S_0 and S_1 states in nonpolar dichloromethane solvent.

1. A (S_0)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-4.938717	0.983843	0.000631
6	0	-5.049757	-0.414956	0.00002
6	0	-3.928193	-1.237082	-0.000459
6	0	-2.684239	-0.611567	-0.000315
6	0	-2.600384	0.782305	0.000298
6	0	-3.69828	1.619366	0.000796
7	0	-1.387264	-1.118458	-0.000706
6	0	-0.606354	-0.074866	-0.000294
8	0	-1.265088	1.121183	0.000339
6	0	0.841466	-0.09187	-0.00048
6	0	1.516343	-1.342734	-0.000209
6	0	2.924051	-1.395808	0.000599
6	0	3.620797	-0.200047	0.000605
6	0	2.971372	1.045104	-0.000036
6	0	1.581131	1.088379	-0.000529
8	0	0.853795	-2.507816	-0.00071
6	0	3.618249	-2.729105	0.000935
6	0	3.769823	2.276045	-0.000224
8	0	3.319963	3.408147	-0.000471
1	0	-5.838235	1.585754	0.000983
1	0	-6.035199	-0.86285	-0.000081
1	0	-4.013764	-2.315513	-0.000915
1	0	-3.60207	2.696327	0.00128
1	0	4.705446	-0.225064	0.001308
1	0	1.077067	2.045358	-0.000895
1	0	-0.122597	-2.328005	-0.000854
1	0	3.341784	-3.318331	-0.876462
1	0	4.69985	-2.598895	0.001679
1	0	3.340508	-3.318694	0.877652
1	0	4.86486	2.114956	-0.000033

2. A (S_1)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	-4.949448	0.986463	-0.00018
6	0	-5.049514	-0.421357	-0.000168
6	0	-3.932508	-1.237777	-0.000087
6	0	-2.668888	-0.60651	-0.000016
6	0	-2.60166	0.820858	-0.000037
6	0	-3.705648	1.636512	-0.000108

7	0	-1.41645	-1.101757	0.000101
6	0	-0.585428	-0.022754	0.000128
8	0	-1.285107	1.183679	0.000063
6	0	0.805006	-0.041645	0.000015
6	0	1.485854	-1.337415	0.000015
6	0	2.892404	-1.434461	0.000097
6	0	3.623525	-0.2539	0.000096
6	0	2.997708	1.01296	0.000039
6	0	1.609977	1.130282	-0.000035
8	0	0.789418	-2.459106	-0.000069
6	0	3.544721	-2.787299	0.00011
6	0	3.864059	2.199776	0.000038
8	0	3.460065	3.353126	0.000018
1	0	-5.85434	1.579926	-0.000242
1	0	-6.034724	-0.870257	-0.000223
1	0	-4.011452	-2.316295	-0.000075
1	0	-3.622382	2.714477	-0.000112
1	0	4.706647	-0.301192	0.000151
1	0	1.149266	2.106705	-0.000076
1	0	-0.200377	-2.244155	-0.000109
1	0	3.254566	-3.370621	-0.87753
1	0	4.629389	-2.68653	0.00041
1	0	3.254086	-3.370837	0.877442
1	0	4.948495	1.987078	0.000109

3. B (S_0)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-5.166491	-0.490463	0.000057
6	0	-4.969965	0.897761	-0.000379
6	0	-3.693786	1.437058	-0.000554
6	0	-2.597965	0.568899	-0.00029
6	0	-2.80741	-0.824625	0.000162
6	0	-4.089166	-1.366799	0.000327
7	0	-1.269713	0.948581	-0.000423
6	0	-0.452422	-0.067378	-0.000103
16	0	-1.257637	-1.654435	0.000451
6	0	0.998017	0.081567	-0.000091
6	0	1.572913	1.385506	0.000069
6	0	2.972538	1.557707	0.000262
6	0	3.770915	0.428611	0.0002
6	0	3.227804	-0.866234	-0.000051
6	0	1.846103	-1.02368	-0.000206
8	0	0.819497	2.491484	0.00003
6	0	3.547772	2.946717	0.000464
6	0	4.122383	-2.027958	-0.000155

8	0	3.764653	-3.193055	-0.000409
1	0	-6.173314	-0.888134	0.00018
1	0	-5.828782	1.556715	-0.00058
1	0	-3.532716	2.507275	-0.000896
1	0	-4.245141	-2.437367	0.000659
1	0	4.849496	0.546095	0.000321
1	0	1.442322	-2.028711	-0.000416
1	0	-0.14005	2.216614	-0.000341
1	0	4.636644	2.911062	0.000691
1	0	3.219876	3.509817	0.877289
1	0	3.220252	3.509914	-0.876442
1	0	5.200955	-1.779955	0.000031

4. B (S_1)

Atomic Number	Atomic Type	Coordinates (Angstroms)		
		X	Y	Z
6	0	-5.161108	-0.522569	-0.000245
6	0	-4.99254	0.869193	-0.000261
6	0	-3.733902	1.423804	-0.000199
6	0	-2.622586	0.571053	-0.000119
6	0	-2.793821	-0.813241	-0.000102
6	0	-4.073756	-1.368571	-0.000166
7	0	-1.255639	0.993644	-0.000048
6	0	-0.466099	-0.047322	0.000021
16	0	-1.247441	-1.618502	0.000007
6	0	1.017034	0.109342	0.000094
6	0	1.580559	1.393568	0.000089
6	0	2.989637	1.534759	0.000136
6	0	3.782775	0.415156	0.000194
6	0	3.234288	-0.88505	0.000215
6	0	1.855023	-1.012831	0.000176
8	0	0.837829	2.554108	0.00003
6	0	3.586086	2.938146	0.000116
6	0	4.129156	-2.049641	0.000489
8	0	3.665766	-3.272538	-0.000233
1	0	-6.161839	-0.93628	-0.000295
1	0	-5.865071	1.509778	-0.000324
1	0	-3.59242	2.497222	-0.000212
1	0	-4.210997	-2.442644	-0.000153
1	0	4.859658	0.526439	0.000207
1	0	1.41101	-1.999105	0.000183
1	0	-0.109585	2.24867	0.000019
1	0	4.670377	2.892646	0.000142
1	0	3.263449	3.494024	0.877477
1	0	3.263488	3.493983	-0.877285
1	0	5.207214	-1.931536	-0.000545

5. C (S_0)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	5.06125	-0.4908	-0.014237
6	0	5.027059	0.914775	0.016554
6	0	3.826715	1.612989	0.031884
6	0	2.660686	0.853637	0.015297
6	0	2.680108	-0.556605	-0.015444
6	0	3.895836	-1.242979	-0.030618
7	0	1.321796	1.196672	0.022162
6	0	0.593692	0.037402	-0.003405
7	0	1.380609	-1.028279	-0.025965
6	0	-0.861823	-0.043493	-0.004661
6	0	-1.48351	-1.324874	0.002712
6	0	-2.888481	-1.444487	0.011266
6	0	-3.645085	-0.286287	0.00769
6	0	-3.054078	0.986534	-0.004315
6	0	-1.665612	1.092321	-0.010978
8	0	-0.768434	-2.455982	0.002037
6	0	-3.516077	-2.810509	0.022074
6	0	-3.903305	2.179825	-0.010321
8	0	-3.502688	3.331688	-0.021977
1	0	6.020068	-0.993606	-0.025631
1	0	5.958967	1.465759	0.028437
1	0	3.802146	2.69466	0.055117
1	0	3.920567	-2.324835	-0.054486
1	0	0.954869	2.134355	0.052097
1	0	-4.727374	-0.363366	0.013154
1	0	-1.23366	2.084885	-0.023619
1	0	0.205975	-2.214086	-0.010863
1	0	-4.602838	-2.733588	0.030101
1	0	-3.216978	-3.389856	-0.854535
1	0	-3.203457	-3.382118	0.899019
1	0	-4.990412	1.972703	-0.003631

6. C (S_1)				
Atomic	Atomic	Coordinates (Angstroms)		
Number	Type	X	Y	Z
6	0	5.053648	-0.477743	-0.00128
6	0	5.007581	0.941267	0.003168
6	0	3.804302	1.638283	0.005056
6	0	2.643198	0.876377	0.002275
6	0	2.668397	-0.567482	-0.002077
6	0	3.907807	-1.244135	-0.00393
7	0	1.319834	1.210298	0.00254

6	0	0.573608	0.035268	-0.000833
7	0	1.412524	-1.046819	-0.003646
6	0	-0.824084	-0.035911	-0.002224
6	0	-1.45502	-1.330632	-0.000917
6	0	-2.868903	-1.463146	0.001721
6	0	-3.622343	-0.305868	0.00225
6	0	-3.048691	0.99003	-0.000202
6	0	-1.661716	1.135372	-0.003127
8	0	-0.743504	-2.448989	-0.001521
6	0	-3.487617	-2.832475	0.003686
6	0	-3.948861	2.138344	-0.000213
8	0	-3.571744	3.318084	-0.002475
1	0	6.021162	-0.963056	-0.002593
1	0	5.938428	1.493265	0.005089
1	0	3.775336	2.719284	0.008355
1	0	3.941463	-2.325037	-0.007218
1	0	0.945361	2.145716	0.008776
1	0	-4.704567	-0.385869	0.004413
1	0	-1.239186	2.1289	-0.007442
1	0	0.2387	-2.213747	-0.003661
1	0	-4.574669	-2.757545	0.005856
1	0	-3.186149	-3.410213	-0.873962
1	0	-3.182563	-3.409288	0.8807
1	0	-5.025697	1.895174	0.001289